



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:47 AM UTC

PDB ID : 1F4Y / pdb_00001f4y
Title : CRYSTAL STRUCTURE OF AN ANTI-CARBOHYDRATE ANTIBODY
DIRECTED AGAINST VIBRIO CHOLERAЕ O1 IN COMPLEX WITH
ANTIGEN
Authors : Alzari, P.M.; Souchon, H.
Deposited on : 2000-06-10
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

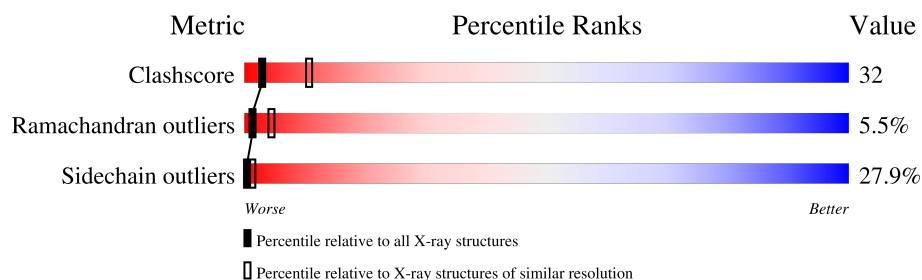
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	210	
2	H	216	
3	A	2	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3231 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

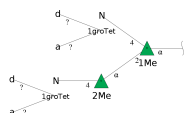
- Molecule 1 is a protein called ANTIBODY S-20-4, FAB FRAGMENT, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	210	Total	C	N	O	S	0	0	0
			1578	989	262	321	6			

- Molecule 2 is a protein called ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1616	1022	262	324	8			

- Molecule 3 is an oligosaccharide called 4,6-dideoxy-4-{[(2R)-2,4-dihydroxybutanoyl]amino}-2-O-methyl- α -D-mannopyranose-(1-2)-methyl 4,6-dideoxy-4-{[(2R)-2,4-dihydroxybutanoyl]amino}- α -D-mannopyranoside.



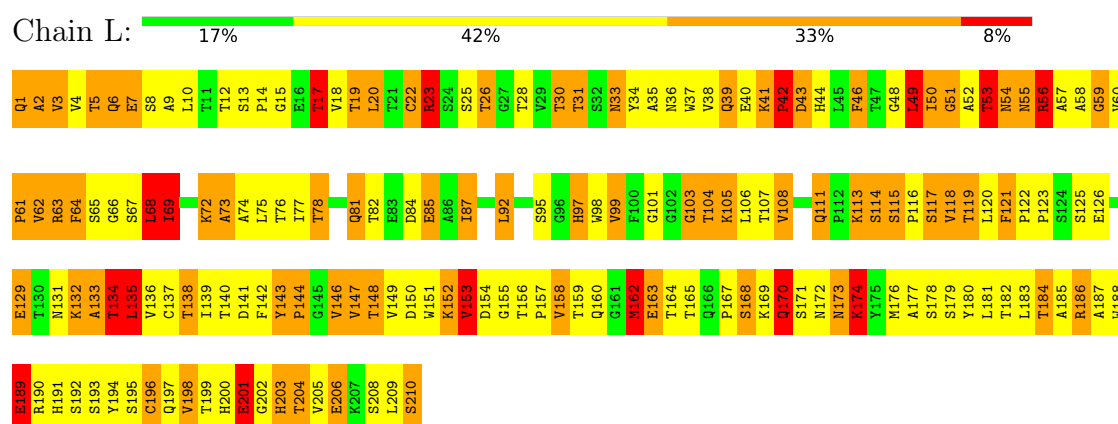
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			37	22	2	13			

3 Residue-property plots

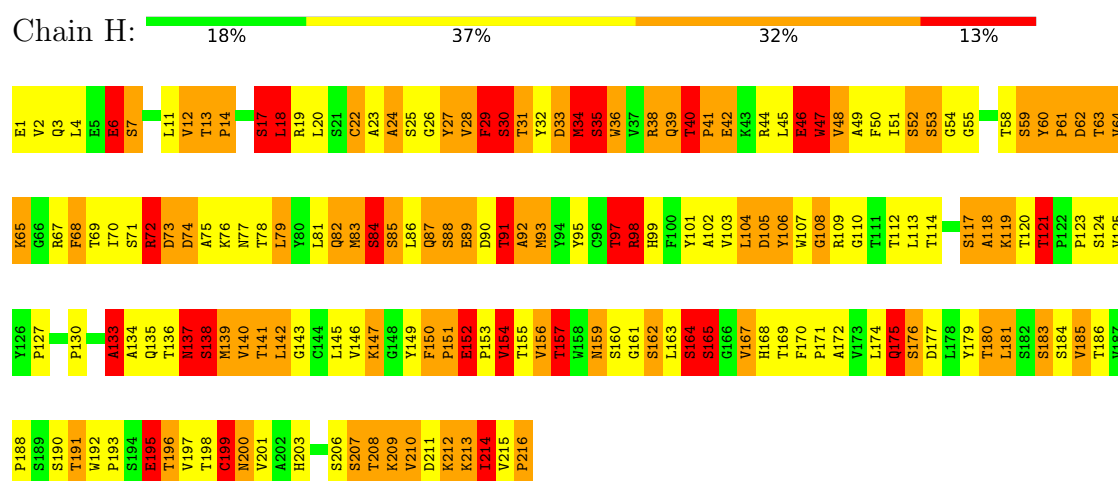
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ANTIBODY S-20-4, FAB FRAGMENT, LIGHT CHAIN



• Molecule 2: ANTIBODY S-20-4, FAB FRAGMENT, HEAVY CHAIN



• Molecule 3: 4,6-dideoxy-4-[(2R)-2,4-dihydroxybutanoyl]amino}-2-O-methyl-alpha-D-mannopyranose-(1-2)-methyl 4,6-dideoxy-4-[(2R)-2,4-dihydroxybutanoyl]amino}-alpha-D-mannopyranoside



ZD01
ZC22

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.69Å 113.36Å 45.58Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.352	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3231	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZD0, ZCZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	L	1.18	0/1615	3.06	203/2208 (9.2%)
2	H	1.25	3/1659 (0.2%)	3.12	206/2272 (9.1%)
All	All	1.21	3/3274 (0.1%)	3.09	409/4480 (9.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
2	H	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	215	VAL	C-O	-5.60	1.17	1.24
2	H	98	ARG	CD-NE	-5.44	1.38	1.46
2	H	216	PRO	N-CD	5.13	1.54	1.47

All (409) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	98	ARG	CD-NE-CZ	33.66	171.52	124.40
1	L	56	ARG	CD-NE-CZ	17.67	149.14	124.40
1	L	55	ASN	CA-CB-CG	15.43	128.03	112.60
1	L	190	ARG	N-CA-C	14.21	126.46	110.97
2	H	2	VAL	N-CA-C	13.72	127.87	109.21
1	L	64	PHE	CA-CB-CG	-13.52	100.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	63	ARG	CD-NE-CZ	13.11	142.76	124.40
1	L	125	SER	CA-CB-OG	12.63	136.37	111.10
2	H	98	ARG	NE-CZ-NH2	-12.50	107.95	119.20
1	L	23	ARG	CA-CB-CG	12.21	138.51	114.10
1	L	101	GLY	CA-C-O	-12.14	105.61	122.36
2	H	195	GLU	CB-CG-CD	11.71	132.51	112.60
1	L	2	ALA	N-CA-C	11.44	130.22	113.40
2	H	1	GLU	CB-CG-CD	11.40	131.99	112.60
1	L	12	THR	CA-C-O	-11.28	108.88	121.51
2	H	98	ARG	NE-CZ-NH1	11.25	132.75	121.50
2	H	61	PRO	CA-C-N	11.05	142.64	121.54
2	H	61	PRO	C-N-CA	11.05	142.64	121.54
1	L	103	GLY	CA-C-N	10.74	137.34	122.19
1	L	103	GLY	C-N-CA	10.74	137.34	122.19
1	L	142	PHE	CA-C-O	10.74	133.01	120.66
2	H	35	SER	N-CA-C	10.74	126.16	109.52
1	L	197	GLN	OE1-CD-NE2	10.72	133.32	122.60
2	H	101	TYR	CA-C-O	10.63	136.48	122.44
1	L	203	HIS	CA-CB-CG	10.52	124.32	113.80
2	H	23	ALA	CA-C-O	10.50	131.54	120.30
2	H	71	SER	CA-C-O	10.28	132.47	121.06
1	L	41	LYS	CA-C-O	10.26	129.83	120.60
1	L	184	THR	CA-C-O	-10.18	110.46	121.56
2	H	14	PRO	CA-C-O	-10.16	109.88	121.36
2	H	29	PHE	O-C-N	-10.09	109.17	122.59
2	H	177	ASP	CA-CB-CG	-10.05	102.55	112.60
1	L	23	ARG	CB-CG-CD	9.84	133.94	111.30
1	L	111	GLN	CB-CG-CD	9.79	129.24	112.60
1	L	28	THR	CA-C-O	-9.75	110.05	121.46
1	L	19	THR	CA-C-O	-9.69	110.16	121.11
2	H	145	LEU	CA-C-N	9.62	135.53	122.93
2	H	145	LEU	C-N-CA	9.62	135.53	122.93
1	L	189	GLU	CA-C-N	9.55	133.25	120.65
1	L	189	GLU	C-N-CA	9.55	133.25	120.65
1	L	191	HIS	CA-C-O	-9.54	111.20	121.98
2	H	215	VAL	O-C-N	9.50	131.93	121.10
2	H	175	GLN	CG-CD-NE2	9.46	130.59	116.40
2	H	110	GLY	CA-C-O	-9.42	115.73	122.23
2	H	164	SER	N-CA-C	-9.40	101.94	113.41
1	L	63	ARG	NE-CZ-NH2	9.37	127.63	119.20
1	L	23	ARG	NE-CZ-NH2	9.35	127.61	119.20
2	H	137	ASN	CA-CB-CG	9.30	121.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	183	SER	CA-C-O	-9.19	110.36	121.11
2	H	47	TRP	CA-C-N	-9.18	113.13	122.77
2	H	47	TRP	C-N-CA	-9.18	113.13	122.77
1	L	50	ILE	CB-CG1-CD1	9.17	133.06	113.80
2	H	58	THR	CA-C-O	9.12	130.44	120.32
2	H	72	ARG	CA-C-N	9.12	138.28	123.33
2	H	72	ARG	C-N-CA	9.12	138.28	123.33
1	L	148	THR	CB-CA-C	9.07	123.48	110.24
2	H	34	MET	N-CA-C	9.04	123.20	108.55
2	H	41	PRO	CA-C-N	9.03	135.80	120.72
2	H	41	PRO	C-N-CA	9.03	135.80	120.72
1	L	2	ALA	CA-C-O	-8.95	106.90	119.96
1	L	191	HIS	CA-CB-CG	-8.95	104.86	113.80
2	H	153	PRO	O-C-N	-8.91	104.17	121.10
1	L	23	ARG	CG-CD-NE	8.84	131.45	112.00
1	L	202	GLY	N-CA-C	-8.83	102.22	114.67
2	H	38	ARG	CA-C-N	8.78	136.39	123.13
2	H	38	ARG	C-N-CA	8.78	136.39	123.13
1	L	98	TRP	CA-C-O	-8.77	110.89	120.36
1	L	9	ALA	CA-C-O	-8.74	110.11	120.43
1	L	152	LYS	CA-CB-CG	8.71	131.52	114.10
1	L	55	ASN	CA-C-O	8.67	130.54	120.49
2	H	74	ASP	CA-CB-CG	-8.64	103.96	112.60
2	H	19	ARG	NE-CZ-NH2	-8.57	111.49	119.20
2	H	172	ALA	O-C-N	8.50	132.48	122.79
2	H	101	TYR	O-C-N	-8.46	113.01	123.33
1	L	121	PHE	CA-CB-CG	8.42	122.22	113.80
1	L	108	VAL	N-CA-C	-8.26	96.22	108.12
2	H	196	THR	O-C-N	-8.22	113.59	123.29
1	L	163	GLU	CB-CG-CD	-8.22	98.63	112.60
1	L	61	PRO	O-C-N	-8.21	112.86	122.71
1	L	190	ARG	O-C-N	-8.21	113.49	122.03
2	H	184	SER	CA-C-O	-8.18	111.87	121.44
2	H	138	SER	CA-C-N	8.13	134.12	122.09
2	H	138	SER	C-N-CA	8.13	134.12	122.09
1	L	97	HIS	CA-CB-CG	-8.03	105.77	113.80
2	H	106	TYR	CB-CA-C	8.03	123.00	109.75
2	H	32	TYR	N-CA-C	7.99	122.10	110.28
1	L	152	LYS	N-CA-CB	7.97	125.40	111.13
1	L	196	CYS	CA-C-N	-7.97	111.76	122.99
1	L	196	CYS	C-N-CA	-7.97	111.76	122.99
2	H	28	VAL	CA-C-O	7.96	130.73	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	78	THR	N-CA-C	7.83	121.37	109.23
1	L	85	GLU	CA-C-O	-7.82	111.71	120.70
1	L	23	ARG	CA-C-O	-7.79	112.09	121.28
2	H	156	VAL	N-CA-C	-7.76	96.84	108.17
1	L	111	GLN	CA-C-O	-7.68	112.96	120.26
2	H	155	THR	CA-C-O	-7.67	112.67	121.72
1	L	147	VAL	CA-C-O	7.66	129.23	121.49
1	L	97	HIS	CA-C-O	-7.66	113.13	121.94
2	H	29	PHE	CA-CB-CG	-7.65	106.15	113.80
1	L	98	TRP	N-CA-CB	7.62	123.49	110.68
1	L	78	THR	CA-C-O	-7.62	111.94	120.32
1	L	134	THR	O-C-N	7.61	132.54	123.33
1	L	19	THR	CA-C-N	7.60	135.10	122.33
1	L	19	THR	C-N-CA	7.60	135.10	122.33
1	L	56	ARG	O-C-N	-7.59	113.59	122.93
2	H	52	SER	CA-C-N	7.58	132.19	120.82
2	H	52	SER	C-N-CA	7.58	132.19	120.82
2	H	73	ASP	CA-CB-CG	-7.57	105.03	112.60
2	H	164	SER	CB-CA-C	7.55	122.44	109.24
2	H	79	LEU	CA-C-O	7.53	128.64	120.43
1	L	69	ILE	CA-C-O	7.53	128.41	120.51
1	L	154	ASP	CA-CB-CG	7.53	120.12	112.60
2	H	47	TRP	CA-C-O	7.52	129.56	120.92
1	L	23	ARG	CD-NE-CZ	7.49	134.88	124.40
1	L	141	ASP	CA-CB-CG	-7.48	105.12	112.60
2	H	42	GLU	CA-C-O	7.48	128.58	119.38
2	H	79	LEU	O-C-N	-7.47	114.83	123.27
2	H	47	TRP	CB-CA-C	7.43	121.78	109.53
1	L	41	LYS	CA-C-N	7.41	129.10	119.84
1	L	41	LYS	C-N-CA	7.41	129.10	119.84
1	L	97	HIS	N-CA-C	7.37	120.04	110.53
2	H	79	LEU	CB-CA-C	7.34	121.85	109.75
1	L	58	ALA	CA-C-O	7.31	129.35	121.16
2	H	125	VAL	CA-C-O	7.21	127.96	120.39
2	H	212	LYS	CA-C-N	7.19	131.78	121.50
2	H	212	LYS	C-N-CA	7.19	131.78	121.50
1	L	72	LYS	CA-CB-CG	7.14	128.39	114.10
1	L	8	SER	N-CA-C	-7.14	104.70	113.41
2	H	196	THR	CA-C-O	7.12	128.15	120.38
2	H	44	ARG	CB-CG-CD	7.11	127.66	111.30
1	L	184	THR	N-CA-C	-7.08	100.51	110.50
2	H	101	TYR	N-CA-C	-7.07	102.63	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	47	TRP	O-C-N	-7.06	114.97	123.16
2	H	99	HIS	CB-CA-C	-7.05	99.14	111.05
2	H	152	GLU	CB-CG-CD	7.05	124.58	112.60
2	H	154	VAL	N-CA-CB	7.03	124.00	111.63
2	H	124	SER	CB-CA-C	7.02	122.78	109.37
1	L	77	ILE	N-CA-C	-7.01	95.05	107.18
1	L	81	GLN	OE1-CD-NE2	7.00	129.60	122.60
2	H	23	ALA	N-CA-C	6.99	119.81	108.41
2	H	32	TYR	CA-C-N	6.95	133.61	120.97
2	H	32	TYR	C-N-CA	6.95	133.61	120.97
2	H	31	THR	N-CA-CB	-6.93	99.28	109.82
1	L	6	GLN	O-C-N	-6.93	115.50	123.33
1	L	61	PRO	CA-C-O	6.93	132.29	122.31
1	L	105	LYS	N-CA-CB	6.91	120.50	110.06
1	L	2	ALA	CA-C-N	-6.87	114.24	123.10
1	L	2	ALA	C-N-CA	-6.87	114.24	123.10
2	H	183	SER	CA-C-N	-6.87	111.81	122.59
2	H	183	SER	C-N-CA	-6.87	111.81	122.59
2	H	46	GLU	N-CA-CB	6.86	123.54	111.13
2	H	27	TYR	CA-CB-CG	6.84	126.21	113.90
2	H	52	SER	N-CA-CB	6.84	120.81	110.42
1	L	63	ARG	CA-C-O	-6.83	113.31	120.55
1	L	99	VAL	CA-C-O	-6.83	113.22	120.53
2	H	47	TRP	N-CA-CB	-6.82	99.18	110.23
1	L	49	LEU	N-CA-CB	6.81	122.00	110.49
2	H	108	GLY	O-C-N	-6.81	115.58	122.59
2	H	72	ARG	NH1-CZ-NH2	6.80	128.15	119.30
2	H	97	THR	N-CA-CB	6.80	122.24	110.81
1	L	170	GLN	CA-C-O	6.79	130.22	120.51
1	L	84	ASP	CA-C-O	-6.79	110.42	119.11
1	L	76	THR	N-CA-CB	6.78	121.70	110.85
1	L	173	ASN	CB-CA-C	6.78	121.52	111.89
2	H	2	VAL	CA-C-O	6.78	129.17	121.11
2	H	101	TYR	CA-CB-CG	6.78	126.10	113.90
2	H	30	SER	CA-C-O	6.72	127.62	120.70
1	L	147	VAL	CA-C-N	6.71	132.46	121.86
1	L	147	VAL	C-N-CA	6.71	132.46	121.86
2	H	157	THR	CB-CA-C	6.68	123.35	109.38
1	L	148	THR	CA-CB-OG1	-6.67	99.59	109.60
1	L	31	THR	CA-CB-OG1	6.67	119.60	109.60
2	H	195	GLU	CA-C-N	6.66	132.19	123.00
2	H	195	GLU	C-N-CA	6.66	132.19	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	36	ASN	CA-CB-CG	6.66	119.26	112.60
2	H	26	GLY	CA-C-O	-6.65	109.00	120.57
2	H	32	TYR	CA-C-O	6.65	128.60	121.16
2	H	65	LYS	CA-CB-CG	6.64	127.37	114.10
1	L	129	GLU	CA-C-O	-6.63	112.77	120.20
2	H	140	VAL	O-C-N	6.61	130.62	123.03
1	L	126	GLU	CB-CA-C	-6.60	100.79	110.96
1	L	135	LEU	CA-C-O	6.59	127.82	120.70
1	L	168	SER	CB-CA-C	6.58	121.17	109.65
2	H	17	SER	CA-C-O	-6.58	114.38	121.36
1	L	20	LEU	O-C-N	-6.56	115.35	123.36
1	L	107	THR	CA-C-O	-6.55	113.53	120.80
1	L	146	VAL	CB-CA-C	6.53	120.56	110.50
2	H	172	ALA	CA-C-O	-6.51	114.32	121.87
2	H	48	VAL	CA-CB-CG2	6.50	121.46	110.40
1	L	185	ALA	O-C-N	-6.50	113.95	122.39
1	L	129	GLU	O-C-N	-6.49	114.80	122.20
1	L	150	ASP	CA-CB-CG	6.49	119.09	112.60
2	H	212	LYS	CA-C-O	6.49	127.29	120.54
1	L	111	GLN	CG-CD-NE2	-6.47	106.69	116.40
1	L	87	ILE	N-CA-CB	6.44	118.72	110.99
2	H	99	HIS	CA-C-O	-6.44	114.02	120.98
1	L	87	ILE	CA-CB-CG1	6.44	121.34	110.40
2	H	161	GLY	O-C-N	-6.42	114.35	122.70
1	L	158	VAL	CA-C-O	-6.42	113.19	120.95
2	H	86	LEU	CA-C-O	6.40	128.34	121.55
2	H	143	GLY	CA-C-O	-6.40	115.33	121.41
2	H	36	TRP	CA-C-O	6.38	127.33	120.38
1	L	204	THR	CA-C-O	-6.37	113.31	120.32
2	H	58	THR	O-C-N	-6.36	115.87	123.31
1	L	119	THR	CB-CA-C	6.36	119.63	110.79
2	H	120	THR	CA-CB-OG1	-6.34	100.09	109.60
2	H	12	VAL	CB-CA-C	-6.34	100.89	111.29
2	H	30	SER	N-CA-C	6.34	117.98	111.14
1	L	151	TRP	CA-C-N	-6.33	111.47	122.37
1	L	151	TRP	C-N-CA	-6.33	111.47	122.37
2	H	45	LEU	CA-C-O	-6.32	114.01	120.71
2	H	61	PRO	O-C-N	-6.31	114.12	122.64
2	H	106	TYR	CB-CG-CD2	6.29	130.24	120.80
1	L	61	PRO	CA-C-N	6.29	128.48	120.56
1	L	61	PRO	C-N-CA	6.29	128.48	120.56
2	H	71	SER	O-C-N	-6.28	117.75	123.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	114	SER	CB-CA-C	-6.28	98.66	110.16
2	H	147	LYS	CA-C-N	6.27	131.67	121.00
2	H	147	LYS	C-N-CA	6.27	131.67	121.00
2	H	60	TYR	CA-C-O	6.24	126.08	120.34
2	H	36	TRP	N-CA-CB	6.21	120.32	110.57
2	H	62	ASP	N-CA-C	6.19	123.99	110.80
2	H	175	GLN	CG-CD-OE1	-6.19	108.42	120.80
1	L	209	LEU	CA-C-O	-6.18	114.65	121.33
2	H	159	ASN	OD1-CG-ND2	6.17	128.77	122.60
2	H	30	SER	CA-C-N	6.16	129.36	120.79
2	H	30	SER	C-N-CA	6.16	129.36	120.79
2	H	165	SER	CA-CB-OG	6.16	123.43	111.10
2	H	95	TYR	CB-CA-C	-6.16	97.19	109.33
2	H	199	CYS	CA-C-O	6.16	126.77	120.24
2	H	108	GLY	CA-C-O	6.16	130.57	122.75
1	L	126	GLU	N-CA-CB	6.13	118.86	109.91
1	L	26	THR	O-C-N	6.12	130.53	122.33
1	L	39	GLN	CA-C-O	-6.11	113.77	120.43
1	L	108	VAL	CA-C-O	-6.10	113.90	120.36
1	L	163	GLU	CA-C-O	6.08	127.56	120.14
2	H	133	ALA	CA-C-N	6.08	133.15	121.54
2	H	133	ALA	C-N-CA	6.08	133.15	121.54
1	L	141	ASP	N-CA-C	6.06	120.04	111.92
1	L	111	GLN	CG-CD-OE1	6.06	132.92	120.80
1	L	55	ASN	O-C-N	-6.05	115.57	123.02
2	H	109	ARG	N-CA-C	-6.04	104.62	112.23
1	L	159	THR	CA-C-O	6.03	127.07	119.95
2	H	190	SER	O-C-N	-6.03	116.25	122.64
2	H	177	ASP	CA-C-O	-6.02	111.90	120.51
2	H	154	VAL	N-CA-C	-6.02	100.03	108.27
2	H	32	TYR	O-C-N	-6.01	115.55	122.89
1	L	54	ASN	CA-CB-CG	-6.01	106.59	112.60
2	H	84	SER	CA-C-O	-6.01	114.52	121.49
2	H	97	THR	CB-CA-C	-6.00	99.16	109.65
2	H	105	ASP	CA-C-O	5.99	126.56	119.67
1	L	199	THR	CA-CB-OG1	-5.98	100.62	109.60
1	L	143	TYR	CA-CB-CG	-5.97	103.14	113.90
2	H	119	LYS	CA-CB-CG	5.95	126.00	114.10
2	H	147	LYS	CB-CG-CD	5.94	124.96	111.30
2	H	214	ILE	N-CA-CB	5.93	118.15	111.21
1	L	138	THR	CA-C-O	5.93	126.71	120.54
1	L	2	ALA	N-CA-CB	-5.93	102.73	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	211	ASP	CB-CG-OD1	-5.93	104.77	118.40
1	L	189	GLU	CB-CG-CD	5.92	122.66	112.60
2	H	30	SER	N-CA-CB	-5.92	101.49	110.07
2	H	101	TYR	CB-CA-C	5.91	122.61	112.27
1	L	22	CYS	CA-C-N	5.91	132.68	122.64
1	L	22	CYS	C-N-CA	5.91	132.68	122.64
1	L	62	VAL	N-CA-C	5.90	116.08	110.42
1	L	31	THR	N-CA-CB	5.88	119.68	110.46
1	L	97	HIS	N-CA-CB	-5.88	102.04	110.44
1	L	153	VAL	CB-CA-C	-5.86	102.41	110.96
2	H	93	MET	CA-C-O	-5.85	114.08	120.81
2	H	167	VAL	CA-C-O	-5.85	114.60	121.80
2	H	13	THR	CA-CB-CG2	5.85	120.45	110.50
1	L	210	SER	CA-CB-OG	5.84	122.78	111.10
1	L	115	SER	CA-CB-OG	-5.84	99.43	111.10
2	H	184	SER	O-C-N	5.83	130.74	123.15
2	H	97	THR	CA-CB-OG1	5.83	118.35	109.60
1	L	154	ASP	CA-C-O	5.82	129.36	122.14
2	H	133	ALA	O-C-N	-5.81	114.86	122.59
1	L	115	SER	N-CA-CB	-5.81	101.63	109.88
1	L	121	PHE	N-CA-C	5.81	118.92	110.14
2	H	188	PRO	CA-C-O	5.80	127.96	121.34
2	H	72	ARG	NE-CZ-NH2	-5.79	113.99	119.20
2	H	63	THR	CA-C-O	5.77	126.19	119.32
2	H	97	THR	CA-CB-CG2	-5.76	100.70	110.50
2	H	155	THR	N-CA-C	-5.76	102.00	110.52
2	H	155	THR	N-CA-CB	-5.75	101.25	110.46
2	H	91	THR	CA-CB-OG1	5.75	118.23	109.60
2	H	152	GLU	CA-CB-CG	5.75	125.60	114.10
2	H	168	HIS	CA-C-O	-5.75	112.45	120.21
2	H	210	VAL	CA-C-O	-5.73	114.64	121.28
2	H	180	THR	N-CA-CB	5.72	120.47	111.20
1	L	198	VAL	N-CA-CB	5.71	119.06	111.64
2	H	210	VAL	CB-CA-C	5.69	119.79	110.69
1	L	67	SER	CA-CB-OG	5.68	122.45	111.10
2	H	17	SER	O-C-N	5.67	129.55	122.92
2	H	147	LYS	N-CA-C	5.66	118.63	109.40
2	H	6	GLU	CB-CG-CD	5.65	122.20	112.60
2	H	124	SER	N-CA-C	-5.64	100.21	109.40
1	L	50	ILE	CA-CB-CG1	5.63	119.98	110.40
1	L	160	GLN	OE1-CD-NE2	5.63	128.23	122.60
1	L	143	TYR	O-C-N	5.63	127.79	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	7	GLU	N-CA-CB	5.63	120.00	110.49
1	L	53	THR	O-C-N	-5.62	115.12	122.59
2	H	147	LYS	N-CA-CB	-5.62	101.05	110.83
1	L	177	ALA	CA-C-O	5.61	127.06	120.89
2	H	161	GLY	CA-C-O	5.61	130.33	120.57
1	L	5	THR	N-CA-CB	5.60	119.48	110.85
2	H	185	VAL	CA-CB-CG1	5.60	119.93	110.40
1	L	171	SER	N-CA-C	-5.59	105.27	111.36
2	H	183	SER	O-C-N	5.59	130.11	123.24
1	L	77	ILE	N-CA-CB	5.58	119.60	112.34
2	H	200	ASN	CA-C-O	-5.58	114.24	120.54
1	L	118	VAL	O-C-N	-5.56	116.62	122.57
2	H	41	PRO	CA-C-O	5.56	128.00	119.55
1	L	8	SER	CB-CA-C	5.56	118.97	109.24
1	L	59	GLY	N-CA-C	-5.56	106.83	114.67
1	L	125	SER	N-CA-CB	5.56	118.22	109.94
1	L	87	ILE	CB-CA-C	-5.55	103.29	110.84
1	L	143	TYR	CA-C-O	-5.55	112.55	120.16
2	H	78	THR	CA-C-N	-5.55	115.07	122.72
2	H	78	THR	C-N-CA	-5.55	115.07	122.72
1	L	141	ASP	N-CA-CB	-5.54	103.76	112.46
2	H	153	PRO	CA-C-N	5.54	131.20	122.33
2	H	153	PRO	C-N-CA	5.54	131.20	122.33
2	H	64	VAL	O-C-N	5.53	129.49	122.57
2	H	162	SER	N-CA-CB	-5.53	101.15	110.49
1	L	146	VAL	O-C-N	-5.52	117.19	123.10
1	L	167	PRO	CB-CA-C	5.52	118.46	111.39
1	L	198	VAL	CB-CA-C	-5.52	102.93	110.77
1	L	144	PRO	CA-C-N	5.52	132.23	121.41
1	L	144	PRO	C-N-CA	5.52	132.23	121.41
2	H	92	ALA	CA-C-O	-5.48	115.57	121.38
1	L	67	SER	N-CA-CB	5.47	119.88	111.46
2	H	65	LYS	CG-CD-CE	5.47	123.87	111.30
1	L	104	THR	CA-C-O	-5.46	114.37	120.54
1	L	111	GLN	CA-CB-CG	5.46	125.01	114.10
2	H	150	PHE	N-CA-CB	5.44	120.06	110.37
1	L	56	ARG	CA-C-O	5.43	127.06	120.81
1	L	118	VAL	N-CA-C	-5.43	102.58	109.80
1	L	131	ASN	CB-CG-ND2	5.42	124.54	116.40
2	H	23	ALA	N-CA-CB	-5.41	102.20	110.65
1	L	23	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	L	46	PHE	O-C-N	-5.40	116.89	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	42	PRO	CA-N-CD	-5.40	104.44	112.00
2	H	177	ASP	N-CA-C	5.39	122.28	110.80
1	L	77	ILE	O-C-N	5.39	127.82	122.97
2	H	29	PHE	CB-CA-C	5.38	121.13	110.42
2	H	89	GLU	N-CA-C	-5.38	105.42	111.28
1	L	133	ALA	O-C-N	5.37	129.85	123.24
1	L	17	THR	CA-CB-CG2	5.37	119.63	110.50
1	L	68	LEU	N-CA-C	-5.36	100.45	109.07
2	H	34	MET	N-CA-CB	-5.34	101.53	110.99
1	L	132	LYS	N-CA-CB	5.34	119.64	110.77
1	L	33	ASN	N-CA-CB	5.34	120.13	111.27
2	H	98	ARG	CA-C-O	-5.31	114.54	120.54
1	L	156	THR	CA-C-N	5.31	126.14	119.98
1	L	156	THR	C-N-CA	5.31	126.14	119.98
1	L	121	PHE	CA-C-N	5.31	125.84	120.38
1	L	121	PHE	C-N-CA	5.31	125.84	120.38
1	L	61	PRO	N-CA-C	5.30	118.90	111.33
2	H	121	THR	N-CA-CB	5.30	119.80	110.37
1	L	39	GLN	CB-CA-C	-5.29	101.01	109.75
1	L	131	ASN	OD1-CG-ND2	-5.28	117.32	122.60
2	H	30	SER	CA-CB-OG	-5.28	100.55	111.10
2	H	169	THR	CA-C-O	-5.26	114.95	121.11
2	H	24	ALA	N-CA-C	5.25	117.64	110.55
2	H	123	PRO	CB-CA-C	-5.25	102.90	111.56
1	L	185	ALA	CA-C-N	5.23	131.52	121.54
1	L	185	ALA	C-N-CA	5.23	131.52	121.54
2	H	83	MET	O-C-N	5.23	129.18	123.22
2	H	40	THR	CA-C-N	5.22	125.02	119.28
2	H	40	THR	C-N-CA	5.22	125.02	119.28
2	H	68	PHE	CA-CB-CG	5.22	119.02	113.80
2	H	121	THR	CA-CB-OG1	-5.22	101.78	109.60
1	L	12	THR	O-C-N	5.21	129.53	122.96
2	H	7	SER	CA-C-O	-5.21	115.57	121.25
1	L	51	GLY	O-C-N	-5.21	119.07	123.60
2	H	44	ARG	CA-C-N	5.21	130.48	122.93
2	H	44	ARG	C-N-CA	5.21	130.48	122.93
2	H	26	GLY	O-C-N	5.20	129.46	122.70
2	H	121	THR	CA-CB-CG2	5.20	119.33	110.50
1	L	1	GLN	CA-CB-CG	5.19	124.48	114.10
1	L	111	GLN	O-C-N	5.19	126.44	121.71
1	L	157	PRO	CA-C-O	-5.19	115.82	121.27
1	L	39	GLN	CG-CD-NE2	5.19	124.18	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	30	THR	CB-CA-C	-5.18	100.82	113.15
2	H	188	PRO	CA-C-N	5.17	131.41	121.54
2	H	188	PRO	C-N-CA	5.17	131.41	121.54
1	L	114	SER	CA-CB-OG	-5.16	100.78	111.10
1	L	174	LYS	CA-C-O	-5.16	115.08	121.06
2	H	44	ARG	O-C-N	-5.14	116.99	122.85
1	L	159	THR	CA-CB-CG2	5.12	119.20	110.50
2	H	74	ASP	OD1-CG-OD2	5.11	135.16	122.90
1	L	49	LEU	O-C-N	5.11	129.38	122.59
1	L	31	THR	N-CA-C	-5.09	107.08	113.28
1	L	97	HIS	CB-CA-C	-5.08	99.88	110.40
1	L	73	ALA	O-C-N	-5.08	116.86	122.86
2	H	45	LEU	N-CA-C	-5.08	101.42	109.59
2	H	27	TYR	N-CA-C	-5.07	100.61	108.42
1	L	183	LEU	CA-C-O	5.07	126.83	121.11
1	L	38	VAL	O-C-N	-5.06	116.75	122.72
1	L	165	THR	CB-CA-C	-5.06	101.19	109.53
2	H	87	GLN	CB-CA-C	5.04	118.37	109.80
1	L	162	MET	CA-CB-CG	5.03	124.17	114.10
1	L	67	SER	CA-C-O	-5.03	116.05	121.38
2	H	162	SER	O-C-N	-5.03	115.90	122.59
2	H	156	VAL	CA-C-O	-5.02	114.96	120.43
1	L	111	GLN	N-CA-C	-5.02	103.70	108.22
1	L	15	GLY	O-C-N	-5.01	117.21	122.52
1	L	19	THR	CA-CB-OG1	-5.00	102.09	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	209	LYS	Mainchain
1	L	117	SER	Mainchain
1	L	174	LYS	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1578	0	1523	92	0
2	H	1616	0	1554	108	0
3	A	37	0	0	7	0
All	All	3231	0	3077	203	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1:ZD0:C5	3:A:1:ZD0:C1M	2.02	1.35
3:A:1:ZD0:C1M	3:A:1:ZD0:C3	2.21	1.17
1:L:41:LYS:HD2	1:L:42:PRO:HD2	1.42	1.02
3:A:1:ZD0:C1M	3:A:1:ZD0:C4	2.40	0.99
2:H:102:ALA:HA	3:A:2:ZCZ:C2M	1.96	0.95
2:H:130:PRO:HD3	2:H:142:LEU:HD12	1.54	0.88
1:L:48:GLY:HA3	2:H:105:ASP:HA	1.59	0.85
1:L:30:THR:HG22	1:L:31:THR:H	1.42	0.83
1:L:123:PRO:HD3	1:L:135:LEU:HD23	1.63	0.80
1:L:123:PRO:HG3	1:L:133:ALA:HB1	1.63	0.80
2:H:97:THR:HG22	2:H:106:TYR:O	1.83	0.78
2:H:51:ILE:HD13	2:H:70:ILE:HG23	1.66	0.78
1:L:5:THR:HG23	1:L:23:ARG:HH22	1.50	0.77
1:L:69:ILE:O	1:L:72:LYS:HB3	1.83	0.77
1:L:63:ARG:HH11	1:L:81:GLN:HG3	1.52	0.75
2:H:157:THR:HG23	2:H:200:ASN:HB2	1.66	0.75
2:H:136:THR:O	2:H:137:ASN:HB3	1.88	0.73
1:L:149:VAL:HG21	1:L:164:THR:HG21	1.71	0.72
1:L:187:ALA:O	1:L:188:TRP:C	2.32	0.72
2:H:47:TRP:HH2	2:H:50:PHE:HB2	1.53	0.71
1:L:200:HIS:O	1:L:201:GLU:HB2	1.89	0.71
2:H:47:TRP:CH2	2:H:50:PHE:HB2	2.25	0.71
1:L:34:TYR:O	1:L:35:ALA:C	2.35	0.70
2:H:27:TYR:CE1	2:H:29:PHE:HA	2.27	0.69
2:H:149:TYR:OH	2:H:181:LEU:HD13	1.94	0.68
2:H:175:GLN:HE21	2:H:175:GLN:HA	1.58	0.68
1:L:63:ARG:HH11	1:L:81:GLN:CG	2.07	0.66
1:L:97:HIS:ND1	1:L:97:HIS:N	2.42	0.66
2:H:137:ASN:O	2:H:139:MET:N	2.28	0.66
2:H:48:VAL:HG13	2:H:64:VAL:HG11	1.77	0.66
1:L:123:PRO:CG	1:L:133:ALA:HB1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:LYS:NZ	1:L:173:ASN:OD1	2.28	0.66
2:H:88:SER:O	2:H:91:THR:HG23	1.96	0.65
2:H:61:PRO:HD2	2:H:64:VAL:CG2	2.26	0.65
2:H:149:TYR:HE1	2:H:152:GLU:HG2	1.61	0.65
1:L:56:ARG:NH1	1:L:62:VAL:O	2.29	0.65
2:H:198:THR:HA	2:H:213:LYS:HA	1.80	0.64
2:H:39:GLN:HE21	2:H:39:GLN:HA	1.63	0.64
1:L:120:LEU:HD13	1:L:196:CYS:HB2	1.79	0.63
1:L:172:ASN:OD1	1:L:174:LYS:HB2	1.99	0.63
2:H:28:VAL:O	2:H:30:SER:N	2.31	0.63
2:H:67:ARG:NH1	2:H:87:GLN:HG2	2.14	0.62
1:L:139:ILE:HG12	1:L:198:VAL:HG21	1.79	0.62
2:H:39:GLN:HE21	2:H:39:GLN:CA	2.10	0.61
2:H:133:ALA:O	2:H:135:GLN:N	2.32	0.61
1:L:113:LYS:HE2	1:L:201:GLU:HG3	1.83	0.61
2:H:20:LEU:HG	2:H:83:MET:HE2	1.82	0.61
2:H:31:THR:O	2:H:53:SER:OG	2.19	0.61
2:H:141:THR:HB	2:H:186:THR:OG1	2.01	0.61
2:H:17:SER:O	2:H:18:LEU:HB2	1.98	0.61
1:L:35:ALA:HB3	1:L:53:THR:HA	1.82	0.60
2:H:98:ARG:HH11	2:H:106:TYR:HD2	1.50	0.60
2:H:34:MET:SD	2:H:79:LEU:HD22	2.42	0.60
1:L:17:THR:OG1	1:L:78:THR:HA	2.01	0.60
1:L:39:GLN:HB2	1:L:49:LEU:HD21	1.84	0.59
1:L:123:PRO:HD3	1:L:135:LEU:CD2	2.31	0.59
1:L:114:SER:OG	1:L:115:SER:N	2.36	0.59
2:H:103:VAL:O	2:H:104:LEU:C	2.46	0.58
2:H:102:ALA:N	3:A:2:ZCZ:O7	2.35	0.58
2:H:206:SER:O	2:H:207:SER:C	2.46	0.58
2:H:103:VAL:O	2:H:105:ASP:N	2.37	0.58
2:H:35:SER:HG	2:H:47:TRP:HZ3	1.53	0.57
1:L:118:VAL:HG13	1:L:137:CYS:SG	2.45	0.57
2:H:52:SER:O	2:H:72:ARG:NH1	2.38	0.56
1:L:5:THR:HG23	1:L:23:ARG:NH2	2.18	0.56
1:L:1:GLN:NE2	1:L:2:ALA:HB2	2.20	0.56
2:H:48:VAL:HG11	2:H:68:PHE:CE2	2.40	0.56
1:L:136:VAL:HG12	1:L:138:THR:HG23	1.88	0.55
2:H:97:THR:HG21	2:H:107:TRP:CE2	2.41	0.55
1:L:50:ILE:HD11	1:L:64:PHE:HB3	1.87	0.55
1:L:63:ARG:NH1	1:L:81:GLN:HG3	2.20	0.55
1:L:42:PRO:O	1:L:43:ASP:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:113:LYS:NZ	1:L:113:LYS:CB	2.70	0.54
1:L:30:THR:HG22	1:L:31:THR:N	2.15	0.54
1:L:56:ARG:HD3	1:L:61:PRO:O	2.08	0.54
2:H:40:THR:HB	2:H:41:PRO:CD	2.37	0.54
2:H:76:LYS:O	2:H:77:ASN:HB2	2.08	0.54
1:L:52:ALA:O	1:L:54:ASN:N	2.41	0.53
2:H:102:ALA:CA	3:A:2:ZCZ:C2M	2.79	0.53
1:L:18:VAL:HG12	1:L:19:THR:O	2.08	0.53
2:H:48:VAL:HG11	2:H:68:PHE:CD2	2.42	0.53
1:L:57:ALA:HB3	1:L:60:VAL:HG23	1.90	0.53
1:L:158:VAL:HG11	1:L:181:LEU:HD13	1.91	0.53
2:H:24:ALA:HB2	2:H:29:PHE:CD1	2.43	0.53
2:H:40:THR:CB	2:H:41:PRO:CD	2.87	0.53
1:L:132:LYS:HD3	1:L:184:THR:HA	1.91	0.53
2:H:84:SER:OG	2:H:85:SER:N	2.42	0.53
2:H:73:ASP:OD1	2:H:75:ALA:HB3	2.08	0.53
2:H:193:PRO:HG3	2:H:216:PRO:HG3	1.90	0.53
1:L:105:LYS:HG2	1:L:106:LEU:N	2.24	0.52
1:L:123:PRO:HB3	1:L:134:THR:H	1.73	0.52
2:H:6:GLU:OE1	2:H:108:GLY:HA3	2.09	0.52
2:H:91:THR:HB	2:H:114:THR:HA	1.91	0.52
2:H:137:ASN:O	2:H:138:SER:C	2.52	0.52
2:H:170:PHE:O	2:H:171:PRO:C	2.53	0.52
1:L:40:GLU:HB2	1:L:46:PHE:CE1	2.45	0.52
2:H:191:THR:O	2:H:195:GLU:HB2	2.10	0.52
2:H:156:VAL:HG11	2:H:183:SER:HB3	1.91	0.51
1:L:153:VAL:HG13	1:L:194:TYR:CE2	2.45	0.51
2:H:47:TRP:HH2	2:H:50:PHE:CB	2.22	0.51
2:H:50:PHE:HB3	2:H:59:SER:HB2	1.93	0.51
1:L:134:THR:OG1	1:L:182:THR:HG22	2.10	0.51
2:H:83:MET:CE	2:H:113:LEU:HD22	2.41	0.51
2:H:203:HIS:HB3	2:H:208:THR:HB	1.93	0.51
1:L:3:VAL:HG12	1:L:23:ARG:HH12	1.76	0.50
1:L:1:GLN:O	1:L:2:ALA:HB3	2.12	0.50
1:L:10:LEU:HD23	1:L:20:LEU:HD22	1.92	0.50
1:L:63:ARG:NH1	1:L:81:GLN:CG	2.75	0.50
2:H:197:VAL:O	2:H:214:ILE:HG12	2.12	0.50
1:L:205:VAL:HG22	1:L:206:GLU:N	2.27	0.49
1:L:201:GLU:OE2	1:L:201:GLU:HA	2.12	0.49
1:L:6:GLN:O	1:L:7:GLU:C	2.54	0.49
2:H:130:PRO:CD	2:H:142:LEU:HD12	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:PRO:O	2:H:64:VAL:HG22	2.13	0.49
1:L:7:GLU:O	1:L:104:THR:OG1	2.25	0.49
1:L:132:LYS:CD	1:L:184:THR:HA	2.43	0.49
2:H:82:GLN:HE21	2:H:82:GLN:HA	1.77	0.49
1:L:113:LYS:HZ2	1:L:113:LYS:HB2	1.78	0.48
2:H:214:ILE:N	2:H:214:ILE:HD13	2.28	0.48
1:L:22:CYS:HB3	1:L:73:ALA:HB3	1.94	0.48
2:H:49:ALA:HB1	2:H:70:ILE:HB	1.94	0.48
2:H:60:TYR:HB3	2:H:61:PRO:HD2	1.96	0.48
2:H:159:ASN:O	2:H:162:SER:HB3	2.13	0.48
1:L:113:LYS:HD2	1:L:144:PRO:HD3	1.95	0.48
2:H:40:THR:OG1	2:H:42:GLU:HB2	2.14	0.48
2:H:175:GLN:O	2:H:176:SER:C	2.57	0.48
1:L:186:ARG:O	1:L:187:ALA:C	2.56	0.48
2:H:208:THR:CG2	2:H:209:LYS:N	2.77	0.48
2:H:117:SER:O	2:H:118:ALA:O	2.32	0.47
2:H:40:THR:HB	2:H:41:PRO:HD2	1.96	0.47
2:H:146:VAL:HG11	2:H:154:VAL:HG21	1.97	0.47
2:H:149:TYR:CE1	2:H:179:TYR:HB2	2.50	0.47
1:L:42:PRO:O	1:L:43:ASP:CB	2.62	0.47
2:H:54:GLY:O	2:H:55:GLY:C	2.57	0.47
1:L:205:VAL:HG22	1:L:206:GLU:H	1.80	0.47
2:H:201:VAL:O	2:H:209:LYS:HA	2.15	0.46
1:L:41:LYS:CD	1:L:42:PRO:HD2	2.29	0.46
2:H:97:THR:CG2	2:H:107:TRP:CD2	2.98	0.46
2:H:167:VAL:HG22	2:H:185:VAL:HG23	1.96	0.46
2:H:150:PHE:CE2	2:H:151:PRO:HB3	2.51	0.46
2:H:139:MET:HA	2:H:139:MET:HE3	1.98	0.46
1:L:19:THR:O	1:L:20:LEU:HD23	2.16	0.46
2:H:3:GLN:HE21	2:H:3:GLN:HA	1.80	0.46
2:H:67:ARG:HH22	2:H:90:ASP:CG	2.23	0.46
2:H:154:VAL:HG23	2:H:156:VAL:HG23	1.97	0.46
2:H:156:VAL:HG11	2:H:183:SER:CB	2.46	0.46
1:L:14:PRO:HG3	1:L:108:VAL:HG12	1.98	0.45
2:H:6:GLU:HB3	2:H:22:CYS:HB2	1.99	0.45
2:H:185:VAL:HG22	2:H:186:THR:N	2.30	0.45
1:L:69:ILE:O	1:L:69:ILE:HG22	2.15	0.45
2:H:20:LEU:CG	2:H:83:MET:HE2	2.46	0.45
1:L:192:SER:O	1:L:210:SER:HA	2.15	0.45
2:H:196:THR:HG23	2:H:213:LYS:HE3	1.98	0.45
2:H:83:MET:HE1	2:H:113:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:TRP:HA	2:H:193:PRO:HA	1.70	0.45
1:L:136:VAL:HG22	1:L:180:TYR:CD1	2.52	0.45
2:H:175:GLN:HA	2:H:175:GLN:NE2	2.28	0.45
1:L:7:GLU:HG2	1:L:10:LEU:HD21	1.99	0.45
1:L:115:SER:HA	1:L:200:HIS:CE1	2.51	0.45
1:L:51:GLY:O	1:L:52:ALA:C	2.59	0.44
2:H:196:THR:HG23	2:H:213:LYS:CE	2.47	0.44
2:H:60:TYR:O	2:H:65:LYS:NZ	2.49	0.44
1:L:59:GLY:O	1:L:60:VAL:C	2.58	0.44
1:L:33:ASN:O	1:L:34:TYR:C	2.60	0.44
1:L:116:PRO:HB3	1:L:139:ILE:HG23	2.00	0.44
2:H:28:VAL:HG12	2:H:30:SER:OG	2.17	0.44
2:H:38:ARG:N	2:H:46:GLU:O	2.47	0.44
3:A:2:ZCZ:C2M	3:A:2:ZCZ:C4	2.97	0.43
1:L:41:LYS:HD2	1:L:42:PRO:CD	2.30	0.43
2:H:33:ASP:OD1	2:H:52:SER:HA	2.18	0.43
2:H:61:PRO:HD2	2:H:64:VAL:HG22	2.00	0.43
1:L:121:PHE:HA	1:L:122:PRO:HD3	1.88	0.43
2:H:119:LYS:O	2:H:121:THR:HG22	2.19	0.43
1:L:113:LYS:NZ	1:L:113:LYS:HB3	2.34	0.43
1:L:57:ALA:HB3	1:L:60:VAL:CG2	2.49	0.42
2:H:198:THR:HG22	2:H:199:CYS:N	2.34	0.42
2:H:47:TRP:CZ3	2:H:50:PHE:HB2	2.53	0.42
1:L:5:THR:OG1	1:L:23:ARG:NH2	2.52	0.42
1:L:188:TRP:O	1:L:189:GLU:C	2.62	0.42
2:H:127:PRO:HB3	2:H:214:ILE:HG23	2.02	0.42
1:L:116:PRO:HD3	1:L:200:HIS:ND1	2.35	0.42
2:H:97:THR:HG21	2:H:107:TRP:CD2	2.55	0.42
2:H:140:VAL:O	2:H:186:THR:HG23	2.20	0.42
1:L:20:LEU:O	1:L:74:ALA:HA	2.20	0.41
1:L:85:GLU:HA	1:L:106:LEU:O	2.20	0.41
2:H:36:TRP:NE1	2:H:81:LEU:HB2	2.35	0.41
2:H:33:ASP:O	2:H:34:MET:HG3	2.20	0.41
2:H:64:VAL:O	2:H:65:LYS:C	2.62	0.41
2:H:159:ASN:O	2:H:160:SER:C	2.62	0.41
1:L:23:ARG:NH1	1:L:25:SER:HB3	2.35	0.41
2:H:164:SER:O	2:H:165:SER:C	2.63	0.41
1:L:143:TYR:HA	1:L:144:PRO:C	2.45	0.41
1:L:4:VAL:HG23	1:L:99:VAL:CG1	2.51	0.41
2:H:3:GLN:O	2:H:4:LEU:HD23	2.20	0.41
2:H:6:GLU:CD	2:H:108:GLY:HA3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:41:LYS:O	1:L:42:PRO:C	2.64	0.41
1:L:37:TRP:CD2	1:L:75:LEU:HB2	2.56	0.40
1:L:162:MET:HA	1:L:180:TYR:O	2.22	0.40
1:L:68:LEU:HD12	1:L:68:LEU:HA	1.75	0.40
1:L:136:VAL:HG22	1:L:180:TYR:CE1	2.56	0.40
2:H:39:GLN:O	2:H:92:ALA:HB1	2.21	0.40
1:L:33:ASN:HB3	1:L:92:LEU:HB3	2.02	0.40
1:L:53:THR:O	1:L:66:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	208/210 (99%)	178 (86%)	20 (10%)	10 (5%)	2	6
2	H	214/216 (99%)	179 (84%)	22 (10%)	13 (6%)	1	3
All	All	422/426 (99%)	357 (85%)	42 (10%)	23 (6%)	1	4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	43	ASP
1	L	53	THR
1	L	103	GLY
2	H	29	PHE
2	H	62	ASP
2	H	118	ALA
2	H	134	ALA
2	H	138	SER
2	H	165	SER
1	L	42	PRO

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Mol	Chain	Res	Type
1	L	186	ARG
1	L	201	GLU
2	H	104	LEU
2	H	133	ALA
2	H	137	ASN
2	H	191	THR
1	L	95	SER
1	L	155	GLY
1	L	44	HIS
1	L	170	GLN
2	H	18	LEU
2	H	176	SER
2	H	88	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	176/177 (99%)	134 (76%)	42 (24%)	1	3
2	H	182/186 (98%)	124 (68%)	58 (32%)	0	1
All	All	358/363 (99%)	258 (72%)	100 (28%)	0	1

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	13	SER
1	L	17	THR
1	L	23	ARG
1	L	26	THR
1	L	49	LEU
1	L	55	ASN
1	L	56	ARG
1	L	65	SER
1	L	68	LEU

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Mol	Chain	Res	Type
1	L	69	ILE
1	L	82	THR
1	L	87	ILE
1	L	92	LEU
1	L	111	GLN
1	L	113	LYS
1	L	117	SER
1	L	119	THR
1	L	129	GLU
1	L	134	THR
1	L	135	LEU
1	L	140	THR
1	L	146	VAL
1	L	147	VAL
1	L	148	THR
1	L	152	LYS
1	L	153	VAL
1	L	162	MET
1	L	163	GLU
1	L	168	SER
1	L	170	GLN
1	L	176	MET
1	L	178	SER
1	L	179	SER
1	L	189	GLU
1	L	193	SER
1	L	195	SER
1	L	201	GLU
1	L	203	HIS
1	L	204	THR
1	L	206	GLU
1	L	208	SER
2	H	6	GLU
2	H	7	SER
2	H	11	LEU
2	H	12	VAL
2	H	13	THR
2	H	14	PRO
2	H	17	SER
2	H	18	LEU
2	H	22	CYS
2	H	25	SER

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Mol	Chain	Res	Type
2	H	30	SER
2	H	33	ASP
2	H	34	MET
2	H	35	SER
2	H	39	GLN
2	H	40	THR
2	H	46	GLU
2	H	47	TRP
2	H	53	SER
2	H	59	SER
2	H	63	THR
2	H	69	THR
2	H	72	ARG
2	H	74	ASP
2	H	82	GLN
2	H	84	SER
2	H	85	SER
2	H	89	GLU
2	H	91	THR
2	H	93	MET
2	H	97	THR
2	H	98	ARG
2	H	112	THR
2	H	117	SER
2	H	121	THR
2	H	137	ASN
2	H	139	MET
2	H	141	THR
2	H	142	LEU
2	H	147	LYS
2	H	151	PRO
2	H	152	GLU
2	H	154	VAL
2	H	157	THR
2	H	163	LEU
2	H	164	SER
2	H	174	LEU
2	H	175	GLN
2	H	180	THR
2	H	181	LEU
2	H	195	GLU
2	H	199	CYS

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Mol	Chain	Res	Type
2	H	207	SER
2	H	208	THR
2	H	210	VAL
2	H	212	LYS
2	H	213	LYS
2	H	214	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	55	ASN
1	L	111	GLN
2	H	3	GLN
2	H	39	GLN
2	H	82	GLN
2	H	175	GLN
2	H	203	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ZD0	A	1	3	19,19,19	0.91	1 (5%)	22,26,26	3.15	11 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ZCZ	A	2	3	18,18,19	1.22	1 (5%)	17,24,26	4.07	9 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ZD0	A	1	3	-	6/13/33/33	0/1/1/1
3	ZCZ	A	2	3	-	9/13/30/33	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	ZCZ	C4-N4	3.78	1.51	1.45
3	A	1	ZD0	C4-N4	2.64	1.50	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	ZCZ	O7-C7-N4	-9.56	105.85	122.96
3	A	2	ZCZ	C4-N4-C7	-9.48	108.78	123.20
3	A	1	ZD0	C4-N4-C7	-8.26	110.63	123.20
3	A	1	ZD0	C1-O5-C5	-5.18	104.80	113.63
3	A	2	ZCZ	O5-C1-C2	5.02	119.68	109.51
3	A	1	ZD0	O5-C5-C6	4.49	116.71	106.74
3	A	1	ZD0	O1-C1-C2	-4.48	102.97	108.14
3	A	2	ZCZ	O7-C7-C8	-4.38	114.14	120.61
3	A	1	ZD0	O3-C3-C4	-4.33	100.97	109.58
3	A	2	ZCZ	O8-C8-C7	3.95	119.28	110.72
3	A	1	ZD0	O7-C7-N4	-3.84	116.08	122.96
3	A	1	ZD0	O3-C3-C2	3.36	118.31	110.38
3	A	1	ZD0	C1M-O1-C1	-3.29	108.26	113.26
3	A	1	ZD0	C6-C5-C4	-3.17	107.76	113.57
3	A	2	ZCZ	C1-O5-C5	2.67	119.27	112.97
3	A	2	ZCZ	O3-C3-C4	2.63	114.82	109.58
3	A	2	ZCZ	O2-C2-C3	2.19	116.79	109.35
3	A	1	ZD0	O5-C1-C2	2.18	114.84	110.37
3	A	2	ZCZ	O8-C8-C9	2.12	114.77	109.14
3	A	1	ZD0	O5-C1-O1	-2.00	106.28	110.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

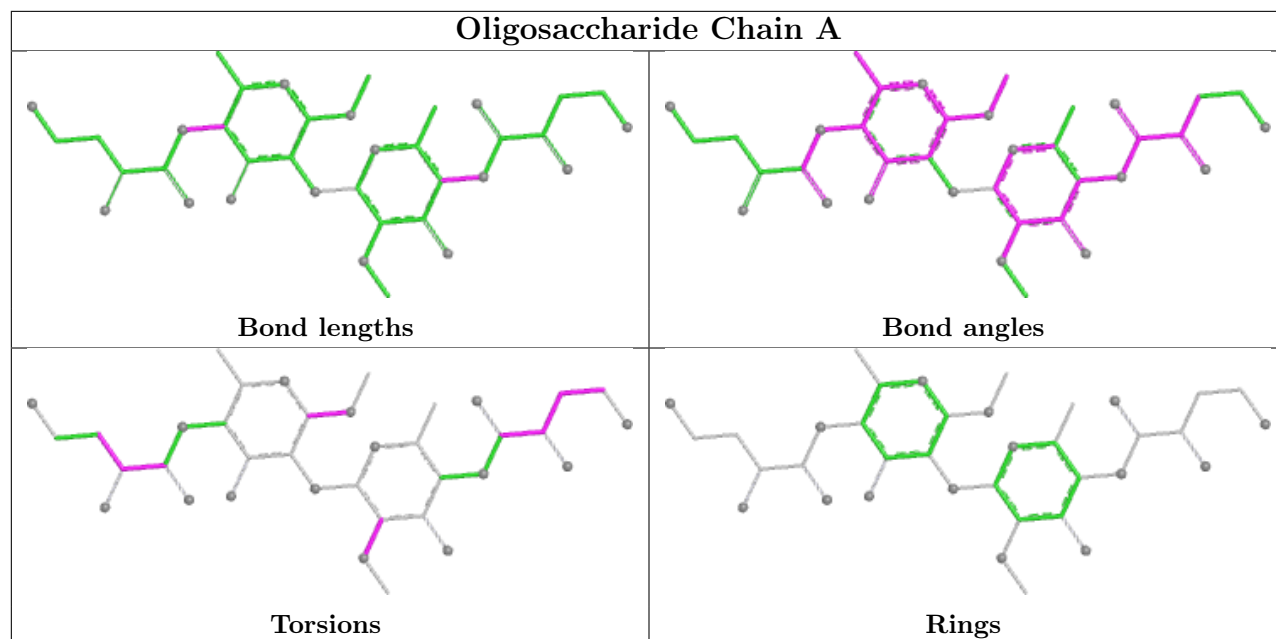
Mol	Chain	Res	Type	Atoms
3	A	1	ZD0	N4-C7-C8-C9
3	A	1	ZD0	N4-C7-C8-O8
3	A	1	ZD0	O7-C7-C8-C9
3	A	1	ZD0	O8-C8-C9-C10
3	A	2	ZCZ	C3-C2-O2-C2M
3	A	2	ZCZ	N4-C7-C8-O8
3	A	2	ZCZ	O7-C7-C8-O8
3	A	2	ZCZ	O8-C8-C9-C10
3	A	2	ZCZ	O10-C10-C9-C8
3	A	1	ZD0	C2-C1-O1-C1M
3	A	2	ZCZ	C7-C8-C9-C10
3	A	1	ZD0	O7-C7-C8-O8
3	A	2	ZCZ	O7-C7-C8-C9
3	A	2	ZCZ	N4-C7-C8-C9
3	A	2	ZCZ	C1-C2-O2-C2M

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	ZCZ	4	0
3	A	1	ZD0	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.